# REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188



| 1. AGENCY USE ONLY (Leave blank) | 2. REPORT DATE | 3. REPORT TYPE AND DATES COVERED |
|---|---|---|
| | 3/24/95 | Final Technical Report for 1/93 - 1/95 |

**4. TITLE AND SUBTITLE**
High Order Accuracy Computational Methods in Aerodynamics Using Parallel Architectures

**5. FUNDING NUMBERS**
F49620-93-1-0090

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**8. PERFORMING ORGANIZATION REPORT NUMBER**
2

AFOSR-TR- 95-0344

**9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)**
Air Force Office of Scientific Research
110 Duncan Avenue, Suite B115
NM Building 410
Bolling AFB, DC 20332

NM

**10. SPONSORING/MONITORING AGENCY REPORT NUMBER**



**11. SUPPLEMENTARY NOTES**

**12a. DISTRIBUTION/AVAILABILITY STATEMENT**
Approved for public release; distribution unlimited.



**13. ABSTRACT** *(Maximum 200 words)*

In this research we presented the development and application of spectral shock cpaturing techniques as well as ENO finite difference and finite element methods for realistic problems. For genuinely time dependent problems, special care had to be taken in order to preserve accuracy. Small errors that do not show up in steady state calculations can be amplified and ruin the total accuracy. Time dependent boundary conditions may also pose problems. We addressed those issues in our research efforts. The recent advent of parallel computers poses a special challenge to the users of high order methods. Issues in parallel computing for the simulations of incompressible and compressible flows has been treated.



| 14. SUBJECT TERMS | 15. NUMBER OF PAGES 17 |
|---|---|
| | 16. PRICE CODE |

| 17. SECURITY CLASSIFICATION OF REPORT | 18. SECURITY CLASSIFICATION OF THIS PAGE | 19. SECURITY CLASSIFICATION OF ABSTRACT | 20. LIMITATION OF ABSTRACT |
|---|---|---|---|
| UNCLASSIFIED | UNCLASSIFIED | UNCLASSIFIED | SAR |

# Final Report AFOSR 93-1-0090
# High Order Accuracy Computational Methods In Aerodynamics Using Parallel Architectures

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**January 1993 - January 1995**

## Abstract

The main theme of this research is the application of high order accurate schemes to complicated flow problems. The advantage of using high order schemes for long time simulations is widely recognized by now. For problems where fine details of the flow field have to be captured accurately the use of high accuracy schemes is mandatory. These two classes of problems encompass many of the current problems in scientific computing.

High order accuracy methods, finite difference , finite elements or spectral methods pose many algorithmic problems. They have less numerical dissipation and therefore they are less robust. In particular when the flow to be simulated includes a shock wave, special treatment has to be given. The famous *Gibbs phenomenon* seems to imply that the presence of the shock wave prohibits the possibility of applying spectral methods for problems with discontinuous solutions. We have shown that this is the wrong interpretation of the Gibbs phenomenon and applied the resolution of this phenomenon in this research effort. Thus in this research we present the development and application of spectral shock capturing techniques as well as ENO finite difference and finite element methods for realistic problems.

For genuinely time dependent problems special care has to be taken in order to preserve the accuracy. Small errors that do not show up in steady state calculations can be amplified and ruin the total accuracy. Time dependent boundary conditions may pose problems. We have addressed those issues in our current efforts.

The recent advent of parallel computers poses a special challenge to the users of high order methods. Issues in parallel computing for the simulations of incompressibly and compressible flows had been treated.

The algorithmic developments took place in parallel to the applications. We concentrated on three main applications: Fuel air mixing enhanced by shock induced vortices, Shock vortex interactions and flow past a blunt body.

This report will be divided into the following parts



Appendix A describes the shock capturing codes applied and their implementation, using vector and parallel computers.

# 1. Spectral shock capturing techniques

The problem in applying spectral methods to shock wave problems is their sensitivity to discontinuities. The presence of shock wave creates theoretical as well as practical difficulties.

Two major theoretical breakthroughs that occured in the last period, may clear the way to the successful implementation of spectral methods in simulating complicated shock waves interactions.

The first development involved the solution of the Gibbs phenomenon. The Gibbs phenomenon is related to the well known fact that the rate of convergence of the sequence of partial sums of the Fourier series representation of a function deteriorates rapidly when the function has discontinuities. In essence the new result says that the first $N$ Fourier coefficients of a piecewise analytic function (a finite number of bounded jump discontinuities is permitted) carries much more information than can be revealed by forming the $N$ th order Fourier partial sum. In fact it has been shown that these $N$ coefficients contain enough information so that one can constructively form an approximation to the unknown piecewise analytic function which is exponentially accurate in $N$. This result had been extended too any polynomial method, such as the commonly used Chebyshev method.

The second development concerns the convergence of spectral methods for non-linear hyperbolic equations. It has been shown that with a suitable addition of (spectrally amall) artificial dissipation the method converges. Moreover it has been shown that the usual filtering technique can be cast in terms of the above analized artficial dissipation.

While the above results create a breakthrough that indicate that high order methods are useful for shock wave calculations, a lot of work has still to be done in making the process efficient. Stabilizing the scheme in an optimal way, and extracting the information in an efficient way have to be further studied.

In a series of papers ([25] - [28]) , we have addressed the issue of the *Gibbs Phenomenon*. In an earlier paper we have shown that an exponentially convergent approximation in the *maximum* norm can be reconstructed from the first $N$ Fourier coefficients of a piecewise analytic function. In [25] we discussed resolution properties of this approximation. In [26] we have extended

the proof to the case of many discontinuities and to the case that the Legendre expansion coefficients are given. In [27] we discussed the case in which we know the first $N$ *Gegenbauer* expansion coefficients of a piecewise analytic function. In [28] we discusses the situation in which we have a good approximation to the *interpolation polynomial* (or trigonometrical polynomial) of a piecewise smooth function.

In [39] It has been shown that when the spectral method is applied (with the appropriate smoothing) to a scalar conservation law the numerical solution indeed converges to the entropy solution. This result was confirmed in [40] where we have applied the techniques developed above to extract exponentially accurate information from spectral discretization of the nonlinear Burgers equation.

## 2. High order ENO schemes

We have been continuing our investigation of ENO schemes using point-flux and TVD Runge-Kutta time discretization formulations in the following directions:

(1) Towards the convergence issues, we have investigated entropy consistency for high order Hermite type finite difference and discontinuous Galerkin methods as a first step. We have been able to obtain [5] a cell entropy inequality for the square entropy, for such high order schemes (no restriction on order of accuracy) without resorting to the help of nonlinear limiters. The result is valid for multi space dimensions with arbitrary triangulations and for any fluxes (no restriction on convexity). This is a significant improvement in obtaining cell entropy inequalities since all the previous work in this direction must either resort to modifications to existing limiters or resort to complicated global analysis, and be restricted to second order accuracy. We plan to continue the investigation towards full convergence proofs;

(2) Application of ENO schemes to combustion problems. The first test case is shock interaction with hydrogen bubbles. Different configuration of bubbles is studied to see the effect of shock interaction. High order accuracy is crucial in this problem due to the detailed structures of the solution behind the shock. This project is on going. Stiff source terms must be treated adequately for future tests;

(3) Comparison of two different formulation of ENO schemes: finite volume vs finite difference. The comparison is performed on problems related to curved boundary, inflow outflow boundary conditions, shocks oblique to the grids, and CPU time. It is found out that finite difference version of ENO scheme (the one based on point values and numerical fluxes of Shu and Osher) is much cheaper to run, and can obtain results comparable to finite volume ENO in most of the test cases.

(4) ENO schemes based on rational function building blocks are being investigated. As a first step we are investigating approximation results. The potential here is that in most rapid transition regions, rational functions approximate the true solution better than polynomials. This project is on going. In [8] , we have performed an extensive comparison of the two formulations of ENO schemes: the cell-averaged version first developed by Harten, Engquist, Osher and Chakravarthy, and the point value version first developed by Shu and Osher. The results indicate that for most test cases, the two formula-

tions of ENO schemes yields the same accuracy whereas the point value ENO scheme is much faster In [38], we have studied positivity preserving finite volume schemes in one and two space dimensions for arbitrary triangulations. The equations we solve are Euler equations of compressible gas, and positivity is preserved for density and pressure. A general framework and examples are provided in this paper. In [41], we have applied the ENO scheme to the equations of viscoelasticity with exponential fading memory. Analytical results about the linearized equation for large time are obtained, and compared with the numerical results. Also, nonlinear simulations for both short time and long time are performed. The numerical method is stable and produces very good shock resolution for long time. In [34] we have proved that the high order discontinuous Galerkin method, using approximate Riemann solvers satisfies a cell entropy inequality for the square entropy, for arbitrary order of accuracy and for arbitrary triangulations in multi space dimensions, with or without using the nonlinear limiters. This compares sharply with similar results for finite difference which can be proven only for much more restricted cases: convex, one dimension, and only for special second order schemes. Related stability issues and numerical aspects are also discussed in [35].

# 3. Parallel computing for high order schemes

## (a) Spectral Elements for incompressible flows

The research objective here is to develop parallel algorithms for computational fluid dynamics (CFD) which will permit solution of incompressible flows with the accuracy and resolution demanded by large eddy simulations (LES) of turbulent flows in complex geometries. The work is subdivided into three principal areas: high-order flexible discretizations, fast multi-level iterative solvers, and implementation of LES modeling technology. *All of this work is being developed within the computational framework of distributed memory architectures which provide a favorable price/performance ratio for this class of problems.*

Our numerical approach is based upon the spectral element method, which retains many of the essential features of global spectral discretizations, namely, rapid (exponential) convergence, minimal numerical dissipation and dispersion per degree-of-freedom, and efficient tensor product factorization of spatial derivative operators. The computational domain is subdivided into large macro-elements and the solution, data, and geometry within each element are expressed in terms of high-order polynomials. The use of a weighted-residual procedure permits a reduction in inter-element continuity requirements from $C^1$ to $C^0$, which in turn leads to a reduction in interprocessor communication. The locally-structured/globally-unstructured, approach of the spectral element discretization is ideally suited to the two-level memory hierarchy associated with distributed memory parallel computers.

The performance of general geometry incompressible codes is largely tied to the speed of the elliptic solver for the pressure; development of fast multilevel iterative solvers is a major focus of our current efforts. Presently, we employ a two-level conjugate gradient based solver which uses deflation to project out the coarse grid modes, thereby reducing the condition number of the underlying iteration matrix. The system is preconditioned by local finite-element based operators which are significantly less expensive to invert than their high-order counterparts. In effect, one can obtain high-order accuracy at low-order cost. We have addressed all of the parallel issues associated with this approach, including the use of an efficient parallel coarse-grid solve,

and are able to compute Navier-Stokes solutions at a resolution of 3 million gridpoints on the 512 node Intel Delta at the rate of 4 minutes per time step (6.5 GFLOPS). To improve upon this result, we are currently developing a preconditioner based upon a Schur-complement formulation for the interface variables. This approach leads not only to better conditioning, but also to reduced degrees-of-freedom, which in turn permits the use of projection techniques in which very good initial guesses can be generated by projecting the residual onto results from previous time steps.

Accurate numerical simulation of many high Reynolds number engineering flows will continue to be limited by resolution requirements for the foreseeable future. However, progress is being made to the point where the combination of high-resolution ( $> 10^6$ gridpoints ) and advanced large-eddy simulation (LES) models will be able to conquer many important problems in the near future. Our goal is to couple the latest LES technology developed within the turbulence community with a general geometry Navier-Stokes code capable of solving these demanding problems.

Because of the large number of degrees-of-freedom involved, effective use of high-performance distributed memory parallel architectures is essential to economic resolution of these problems. Principal parallel issues to be addressed include: development of coarse-grid solve strategies which will remain competitive as the number of processors and dimension of the coarse-grid system continue to increase; and development of optimal communication strategies for the complex subdomain interfaces arising from nonconforming discretizations.

### (b) Spectral methods for compressible flows.

Spectral methods involve the approximation of the unknown solution in terms of global polynomials. This fact make them difficult to implement on parallel computers. A popular method to overcome the limitations of spectral methods is to use multidomain techniques, in which a complex domain is decomposed into several simpler subdomains. This method has been applied successfully to incompressible flows (the Specral-Element technique) or to problems in structural mechanics (the h-p method).

Multidomain spectral methods are suitable for coarse grain parallel computing, each domain is assigned to a different processor.

The main question is: Are multidomain methods efficient? This question has not been yet answered for those methods applied to hyperbolic equations. If we denote by $W(p,N)$ the work involved in approximating $k$ waves using p sub domains (and $N$ points in each domain) to obtain an error of at most $e^{-\epsilon}$, then $W(p,N)$ is minimized if

$$p \sim \frac{\pi k}{\epsilon} \tag{1}$$

Thus the optimal number of subdomain *increases* with the complexity of the problem (or number of waves) but *decreases* if the required accuracy increases. This result may serve as a guideline to the optimal number of subdomain. The formula above can be suitably modified for parallel computers.

A key issue in the application of multidomain spectral methods to the numerical solution of hyperbolic equations is the interface boundary conditions. This leads to the question of the imposition of boundary conditions, both analytic and numerical, in the numerical solutions of *systems* of hyperbolic equations. For truly time dependent problems stability in the classical sense (Lax and G-K-S stability) is not enough. Even stable schemes may exhibit a non-physical growth in time. From a practical point of view, in order to achieve reasonable accuracy for large time, meshes much too fine for the computers available in the foreseeable future are required. In the past methods that preserve *summation-by-parts* property of the differential equation were constructed. Recent attempts to utilize these boundary closures to numerically solve a $2 \times 2$ hyperbolic system have shown that, in certain cases, an unwarranted growth in time still results.

In [23], [7] we have outlined a systematic procedure for designing time-stable, as well as G-K-S stable schemes of high-order accuracy. The new schemes are guaranteed to be time-stable for any hyperbolic system (as long as the system has a bounded energy). We have extended this methodology to Navier Stokes equations in three space dimensions. We have showed that the SAT boundary condition assures the correct behavior as the Reynolds number tends to infinity.

We have carried out ([31], [30]) experiments with the new boundary procedure indicate that there are very suitable for parallel computing. Indeed if one assigns each domain to a different processor then the work can be done completely in parallel. The communication issue is related directly to the interface boundary conditions. With the SAT procedure it seems that

communication time may be reduced. This will be one of the

We also a examined a method to approximate the interface conditions for Chebyshev polynomial approximations to the solutions of parabolic problems, and a smoothing technique is used to calculate the interface conditions for a domain decomposition method. The method uses a polynomial of one less degree than the full approximation to calculate the first derivative so that interface values can be calculated by using only the adjacent subdomains. Theoretical results are given for the consistency of the scheme and practical results are presented. Computational results are given for a fourth order Runge-Kutta method in two dimensions and for an explicit/explicit scheme in both one and two dimensions.

### (c) Parallel implementation of ENO schemes on CM-5

The main cost in ENO schemes is in its logic step in choosing local stencils by comparing divided difference tables of the function. Although great effort has been spent on efficiently vectorizing this part for CRAY supercomputers, due to the inevitable gathering-scattering process, ENO schemes still do not run very fast on CRAY computers. Recently we have been exploring the structure of the ENO algorithm to suit the parallel structure of CM-5. The algorithm has been slightly re-formulated (in a mathematically equivalent way) to reduce communications and to eliminate communications between other than next neighbors, at the price of a slightly increased operation count. Our CM-5 two dimensional ENO code for compressible Euler and Navier-Stokes equations is a magnitude faster than our ENO code on CRAY for a 400x400 grid. Three dimensional code also shows a speed up, although it has not been optimized yet (for three dimensions, storage is a big restriction, and the structure of the program must be modified accordingly). Currently we are trying to improve the CM-5 code and applying it to reactive flows. This research is reviewed in [19], see also Appendix A.

## 4. Fuel air mixing enhanced by shock induced vortices

In designing supersonic combuster for the next generation of supersonic transport, we look for an efficient combuster such that :

- allow better load to weight ratio by carrying less fuel,
- reduce chemical product that contribute to pollution due to incomplete burning of fuel.

One of the technique currently under study in enhancing mixing of a hydrogen jet (fuel) and air (oxidizer) is to allow the existing shock inside the combustion chamber to interact with the hydrogen jet . By doing so, vorticity are generated according to the vorticity equation of the Navier Stokes equation, The pressure gradient of the shock and the density gradient between the air and hydrogen provides an efficient mechanism for vorticity generation along the surface of the hydrogen jet. The vorticity forced the jet to curl up and stressed. The increased surface area allows greater mixing of air and hydrogen where combustion can take place. Even though the problem is three dimensional steady state, it had been argued that the three dimensional steady flow can be directly associated with a corresponding two dimensional unsteady calculation in this particular physical setting.

Numerical simulations are a necessary part of this investigation. For these type of problem, it is important to capture the complex physics with high accuracy. Finite difference scheme , with their inherent dissipative nature for stability reason, can only yields a quantitative result of the flow fields. Often, for long time integration, the loss of accuracy in the earlier stage affect the development of the flow in later time.

In Appendix A we describe two codes for simulating the above problem. A spectral shock capturing code and a finite difference ENO code. We have employed all the theoretical techniques developed in order to run succesfully the codes.

we computed the solution of these problem with various configuration of multiple jets placement. Our preliminary results found that different initial placement of the jets yields distinct final configurations (Moreover, the spectral code is fully capable of capturing the fine scale structure of the interactions, including some that had not been seen in finite difference code. One distinct feature of this calculation is the penetration of an air stream

(heavy fluid) into the hydrogen (light fluid) causing instability that exhibit a mushroom shape structure (See Appendix A). This study can be used to guided researcher in develop fuel jet configuration for the scramjet engine with greater confident. Our goal in this research is to extend this problem to a three dimensional steady and/or unsteady simulation with full chemistry model.

A detailed report [19] describes the codes in detail.

## 5. Shock interacting with vortices

In designing supersonic scramjet engine nozzle, acoustic radiation pattern (sound wave) will be generated by the interaction of shock and vortices according to the linear analysis done by Ribner and Moore . The sound wave will have a significant impact on the design of engine that operated at supercritical nozzle pressure ratios. Moreover, sound wave (noise) generated by supersonic aircraft should be minimized for environmental reason, as it travel over populated land mass. Hence, a better understanding of the mechanism of the shock vortices interaction is important.

The vortex is defined as follow : the tangential velocity profile of the vortex centered at $(x_c, y_c)$ in the polar coordinate is

$$U(r) = \begin{cases} \Gamma r(r_0^{-2} - r_1^{-2}) & 0 \le r \le r_0 < r_1 \\ \Gamma r(r^{-2} - r_1^{-2}) & r_0 \le r \le r_1 \\ 0 & r > r_1 \end{cases}$$

where $r_0 = 0.2$ and $r_1 = 1.0$ unless specified otherwise. This vortex is rotating in a counter-clockwise direction. Hence, the velocity field upstream of the shock becomes

$$\begin{aligned} u &= u_r - U(r)\sin\theta \\ v &= v_r + U(r)\cos\theta \end{aligned}$$

where $\theta = \tan^{-1}\left(\frac{y-y_c}{x-x_c}\right)$.

We used Chebyshev collocation methods to solve the two dimensional Euler gas dynamics equation [14]. Using some standard numerical techniques, the spectral code remains stable and highly efficient. we can computed the solution in less than 10 CPU minutes on a Cray 2 supercomputer with grid size up to 256x256 Chebyshev collocation points. As a test case, a mach 3 shock was propagated through air and impacted with a vortex of strength $\Gamma = 0.25$. After reconstruction of the raw data, we are able to recover the solution that depicted strong acoustic wave propagated downstream with good accuracy when compared with ENO third order scheme.

## 6. Compressible wake flows

We are interested here in numerical simulation of a low Mach number, compressible, viscous flow past a circular cylinder at a moderately low Reynolds number. The unsteady wake generated by the cylinder has been of great interest to computational fluid dynamicisits as well as to theoretical and experimental aerodynamicits. The Reynolds number range between 40 and 1000 has been of particular interest because it spans the transition from steady flow to an unsteady wake flow dominated by the period shedding of vortices from the cylinder. The shedding frequency of this vortices is known theoretically and *all* numerical methods, applied to this problem, obtain this frequency within reasonable accuracy. However, Srinivassan measured (in a wind tunnel experiment) more than one distinct frequency in the shedding regime. In addition to the vortex shedding frequency he found clearly, discernible lower frequencies and concluded that this was a feature of the initial stage of transition to turbulence. A numerical simulation, using the second order accurate MacCormack scheme did find a secondary frequency, very nearly the same found in the wind-tunnel experiment.

We have developed at Brown the most accurate code for this configuration. The code simulates the *axial-symmetric time dependent , compressible viscous Navier-Stokes equations.* It uses Fourier methods in the $\theta$ direction and Chebyshev methods in the radial direction. This code found no secondary frequencies. Spectral methods are , of course, methods with high order accuracy, and as any other high order method, are very sensitive to the kind of outflow boundary conditions treatment. In particular they tolerate only those treatments based on the *characteristic variables.* Low order methods are more tolerant and allow high variety of boundary conditions. When the far field boundary conditions from the spectral code, were incorporated into the second order code, the secondary frequency disappeared. The spurious frequency was generated by a boundary condition that was tolerated by the low order (and robust) MacCormack scheme but not by the high order scheme used. It is interesting to note that when the wind tunnel experiment was repeated in a bigger wind tunnel where effect from the walls were eliminated, the secondary frequency disappeared. The above example illustrates the type of surprises one might encounter when using low order schemes for long time integrations. Stability, in the classical sense of Lax , is not enough anymore, one has to be careful not to have spurious phenomena. It also illus-

trates the fact that the gross features of the flow (in this case the shedding frequency) were obtained even with low order schemes. It is only when some delicate features of the flow were sought for that an unphysical solution had been observed. The fact that the lower order scheme produced a spurious solution does not contradict the fact that the scheme is stable and converges *as the number of grid-points increases.* The spurious solution will eventually disappear if further grid refinements will be carried out. However for realistic grids it is impossible to distinguish between a physical and a spurious solutions. *a high order scheme is less likely to produce a spurious solution.* With this in mind we further investigated delicate physical questions.

**The effect of heating of the cylinder on the shedding.**

This is a fundamental question and there are only few wind tunnel experiments (done by Srinivassan) to indicate the possible effects on the shedding.

**The interaction of acoustic waves with the flow and its effect on the shedding.**

A compact 4-th order and sixth order finite difference scheme has also been incorporated into the spectral code. (See for a description of the code in [20] A detailed analysis of the effects of the heating of the cylinder on the shedding frequency had been studied using the above schemes. It has been found that the shedding frequency decreases when the wire was heated. Experimental work carried out at NASA Langley confirmed the numerical results.

We have also applied spectral multidomain techniques to the same geometry ([30]) in order to be able to port the code easily to parallel computers.

We are now in the process of studying interactions of acoustic waves and heated cylinders. The physical problem is of great interest to experimentalist that have to calibrate their wind tunnel experiments. Since the probes are heated cylinders, the effect of the acoustic waves on them has to be taken into account.

## 7. The efficient implementation of spectral and high order schemes

High order finite difference methods were considered as an alternative to Spectral methods. In [5] a series of compact fourth- and sixth-order schemes were developed and their stability for mixed initial-boundary value problems had been verified using the GKS theory. In [6] The problem of time stability was also addressed and fourth order schemes that satisfy evergy norm were constructed. In [7] we had pointed out that time stability for system *does not follow* from scalar time stability and presented a systematic way for constructing boundary conditions for compact (and spectral) schemes. This is the first work that the issue of time stability for systems has been addressed.

In [7] we have shown that the conventional method of imposing time dependent boundary conditions for Runge-Kutte time advancement reduces the formal accuracy of the space time method to second order. This counter intuitive result was analyzed and a remedy was given for linear problems. A partial remedy had been given for some nonlinear problems in [37] and [1]..

A step between the theory and the applications is the issue of efficient implementation of the theory. Progress had been made in different directions. In [18] the authors studied a new method in reducing the roundoff error in the computations of derivatives by Chebyshev methods. In [17] mappings were considered for Legendre methods. In [15] we constructed a new collocation method that uses Chebyshev points, convenient for the applications, but still has all the theoretical advanatges of the Legendre methods. In [31] we presented a time stable open boundary conditions for the numerical approximation of the Compressible Navier-Stokes equations in 3-D and discussed their implementation within spectral and high order finite difference methods.

## 8. Multiscale Computing

Many relevant physical phenomena involve infinite number of scales. In nonlinear problems it is desirable to find a way to take into account the effect of the scales which are neglected on those which are taken into account.

Two approaches have been investigated for this type of problems: *Nonlinear Galerkin Methods* and *Wavelet based Schemes.*

In [29] we have studied the implementation of the Nonlinear Galerkin in the context of collocation discretizations. We have found interesting characterizations, in the physical space, of a small scale function and a large scale function.

In [13] we presented an efficient pseudospecral NLG scheme for the periodic Burgers equation, The case of Chebyshev approximations to nonperiodic problems, in which the concept of large and small scales have to be redefined is currently under investigation.

In a thesis by L. Jameson and in a subsequent paper [32], the Daubechies wavelet based differentiation matrix was constructed. The relationship between this matrix and finite difference methods was clarified. This serves as a basis for current work by Bruce Bauer a doctoral student on wavelet optimized finite difference methods.

Jameson [33] also analyzed the differentiation matrix based on the compactly supported Daubechies wavelets. He showed that in this case there is a loss of the superconvergence. The same result holds (see [24]) for the finite element schemes.

**List of publications resulting from the grant.**


[1] S. Abarbanel, D. Gottlieb and M. Carpenter , *On the removal of boundary errors caused by Runge-Kutta integration of non-linear partial differential equations* to appear.

[2] R.B. Bauer, *an Efficient Adaptive Grid ENO Scheme*, to appear.

[3] R.B.Bauer, *Band Pass Filters For determining Shock Locations* to appear

[4] W.Cai and C.W. Shu, *Uniform high-Order Spectral Methods for One-and Two-Dimensional Euler Equations* . Journal of Computational Physics, vol 104, No 2 (1993) pp. 427 -443.

[5] M. Carpenter, D. Gottlieb and S. Abarbanel, *The stability of numerical boundary treatments for compact high order finite difference schemes*, Journal of Computational Physics, v108 (1993), pp.272-296.

[6] M. Carpenter, D. Gottlieb and S. Abarbanel, *Stable and accurate boundary treatments for compact, high order finite difference schemes*, Applied Numerical Mathematics, v12 (1993), pp.55-87.

[7] M. Carpenter, D. Gottlieb, S. Abarbanel and W.-S. Don, *The theoretical accuracy of Runge-Kutta time discretizations for the initial boundary value problem: a study of the boundary error*, SIAM Journal on Scientific Computing, to appear.

[8] J. Casper, C.-W. Shu and H. Atkins, *A comparison of two formulations for high-order accurate essentially non-oscillatory schemes*, AIAA Journal, v32 (1994), pp.1970-1977.

[9] B.Cockburn and C.W.Shu, *Nonlinearly Stable Compact Schemes For Shock Calculations*, SIAM Journal of Numerical Analysis, vol 31, No 3, pp 607-627 (1994).

[10] W.E and C.W.Shu, *Effective Equations and the Inverse Cascade Theory for Kolmogorov Flows*, . Phys. Fluids A5(4), (1993) pp. 998-1010.

[11] W.E and C.W.Shu, *Small-Scale structures in Boussinesq convection* Phys.Fluids (1994) pp 49-58

[12] W.E and C.W.Shu, *A Numerical Resolution Study of High Order Essentially Non-oscillatory schemes Applied to Incomprissible Flow.* Journal of Comp.Physics vol.110, No 1, (1994) pp.39-46.

[13] L. Dettori, D. Gottlieb and R. Temam, *A nonLinear Galerkin method: the two-level Fourier-collocation case*, Journal of Scientific Computing, to appear.

[14] W.S. Don, *Numerical study of pseudospectral methods in shock wave applications*, Journal of Computational Physics, v110 (1994), pp.103-111.

[15] W.-S. Don and D. Gottlieb, *The Chebyshev-Legendre method: implementing Legendre methods on Chebyshev points*, SIAM Journal on Numerical Analysis, to appear.

[16] W.-S. Don and A. Solomonoff, *Accuracy and speed in computing the Chebyshev collocation derivative*, SIAM Journal on Scientific Computing, to appear.

[17] W.-S. Don and A. Solomonoff, *Accuracy enhancement for higher derivatives using Chebyshev collocation method and a mapping technique*, SIAM Journal on Scientific Computing, submitted.

[18] W.-S. Don and A. Solomonoff, *A note on the mapping for Legendre collocation methods*, Journal of Computational Physics, to appear.

[19] W.S. Don and C. Quillen , *Numerical simulations of reactive flow, Part I: Resolution* accepted to JCP.

[20] W.S.Don and E.Voth, *High-Order Methods For Two Dimensional Compressible Viscous Flow Around a Circular Cylinder.* to appear.

[21] P.Fischer,F.Preparata,and J.Savage, *Generalized Scans and Tri-Diagonal Systems* to appear in The proceedings of the 12th Symposium on Theoretical Aspects of Computer Science p. 168-180 (1995)

[22] D.Gottlieb, *Issues in the Application of High Order Schemes*, In Algorithmic Trend in CFD (Springer(1993)) pp. 195-215.

[23] D. Gottlieb, S. Abarbanel and M. Carpenter, *Time stable boundary conditions for finite difference schemes solving hyperbolic systems.* Journal of Computational Physics, v111 (1994), pp.220-236.

[24] D. Gottlieb, B. Gustafsson, P. Olsson and B. Strand, *On the superconvergence of Galerkin methods for hyperbolic IBVP*, SIAM Journal on Scientific Computing, to appear.

[25] D. Gottlieb and C.-W. Shu, *Resolution properties of the Fourier method for discontinuous waves*, Computer Methods in Applied Mechanics and Engineering, v116 (1994), pp.27-37.

[26] D. Gottlieb and C.-W. Shu, *On the Gibbs Phenomenon III: recovering exponential accuracy in a sub-interval from a spectral partial sum of a piecewise analytic function*, SIAM Journal on Numerical Analysis, to appear.

[27] D. Gottlieb and C.-W. Shu, *On the Gibbs Phenomenon IV: recovering exponential accuracy in a sub-interval from a Gegenbauer partial sum of a piecewise analytic function*, Mathematics of Computation, to appear.

[28] D. Gottlieb and C.-W. Shu, *On the Gibbs Phenomenon V: recovering exponential accuracy from collocation point values of a piecewise analytic function*, Numerische Mathematik, to appear.

[29] D. Gottlieb and R. Temam, *Implementation of the Nonlinear Galerkin Method with psuedospectral (collocation) discretizations.* Applied Numerical Mathematics, vol 12 (1993), pp.119-134.

[30] J.S.Hesthaven, *Multi Domain Spectral Simulation of Unsteady Compressible flow Around a Circular Cylinder*, To appear.

[31] J.S. Hesthaven and D. Gottlieb, *A stable penalty method For the compressible Navier-Stokes equations, open boundary conditions*, to appear in Siam Journal on Scientific Computing..

[32] L. Jameson, *On the wavelt based differentiation matrix*, Journal of Scientific Computing, v8 (1993), pp.267-305.

[33] L.Jameson , *On The Differentiation Matrix for Spline Wavelets With Periodic Boundary Conditions*, to appear in SINUM.

[34] G. Jiang and C.-W. Shu, *On cell entropy inequality for discontinuous Galerkin methods*, Mathematics of Computation, v62 (1994), pp.531-538.

[35] G. Jiang and C.-W. Shu, *Stability of discontinuous Galerkin methods for general triangulations*, In Developments in Theoretical and Applied Mechanics, Volume XVII, edited by I.C. Jong and F.A. Akl, Louisiana Tech University and University of Arkanas, 1994, pp.227-234.

[36] Martine Marion ,*ON the Stability of Fourier and Legendre Collocation Methods For The Two Dimensional Burgers Equation* To appear in Journal of Scientific Computing.

[37] D. Pathria, *The correct formulation of intermediate boundary conditions for Runge Kutta time integration of initial boundary value problems*, preprint.

[38] B. Perthame and C.-W. Shu, *On positive preserving finite volume schemes for compressible Euler equations*, Numerische Mathematik, to appear.

[39] E. Tadmor, *Super viscosity and spectral approximations of nonlinear conservation laws* to appear.

[40] C.-W. Shu and P. Wong, *A note on the accuracy of spectral method applied to nonlinear conservation laws*, Journal of Scientific Computing, to appear.

[41] C.-W. Shu and Y. Zeng, *High order essentially non-oscillatory scheme for viscoelasticity with fading memory*, Submitted to the Quarterly of Applied Mathematics.

# Appendix A

## 1 Introduction

This research involves study of combustion and mixing induced by the interaction of a shock in air with a hydrogen jets. This model problem is of interest for the design of air-breathing scramjet engines, as it provides a mechanism for inducing millisecond combustion times. Extremely rapid combustion is a necessity in an engine where the reactants are escaping from the reaction chamber at supersonic speeds.

In a pre-mixed combustion process, the combustion rate is limited by the rate at which reactants diffuse across the air-fuel interface. This diffusion rate is determined by the length of the interface and the concentration gradient across it. One way to increase this rate of diffusion is to stretch out the interface by the motion induced from a point vortex [2]. At the same time this would steepen the concentration gradient across the interface by bringing fresh reactants into contact with it. Marble [3] suggests a way to induce this vorticity—to have a shock pass though a jet of fuel nearly perpendicular to its axis. While passing through the region of inhomogeneous density the shock will produce vorticity via the $\frac{\nabla\rho\times\nabla p}{\rho^2}$ term in the vorticity equation:

$$\frac{d\omega}{dt} = (\omega\cdot\nabla)V - \omega\nabla\cdot V + \frac{\nabla\rho\times\nabla p}{\rho^2}.$$

The gradient in pressure across the shock in conjunction with gradient in fluid density between the air and hydrogen produce a large increase in vorticity as the shock passes through the hydrogen jet.

Another factor affecting mixing in this model system is the fluid instability produced as the denser air and lighter hydrogen are accelerated by the shock passing through. This is a similar situation to a heavy fluid lying above a lighter one in a gravitational acceleration. The heavier fluid tends to form fingers descending down into the lighter fluid below, due to the Rayleigh-Taylor instability. A similar instability, the shock-induced Rayleigh-Taylor instability or Richtmyer-Meschkov instability, results in a similar fingering of air into the hydrogen cylinder as the shock passes through.

For this type of problem, it is important to capture the complex physics with high accuracy. Accurate calculations in search of quantitative information about the mixing require high resolution and/or high order schemes. Previous researchers failed to capture many important features of this flow due to the

- inability of their codes to adequately resolve features in the flow [4] [5] [6].
- inherently dissipative nature of the finite difference scheme (FCT [1, 5], for example), which ensured that the computed results were only qualitatively accurate. Often, for long time integration, the loss of accuracy in earlier stages inhibited the development of fine scale features at later times.

According to Marble et al., the 3-D steady shock and profile can be simulated by a 2-D unsteady shock provided several conditions can be met. To make any direct association of the 2-D unsteady flow with the 3-D steady flow in such a geometry, it is required that

- Pressure and Density jumps are matched across the shock.
- The velocity of the feature $(dx/dt|_{2D})$ in 2-D should be related to the corresponding slope $(dz/dx|_{3D})$ in 3-D linearly

$$\frac{1}{c}\frac{dx}{dt}|_{2D} = m\frac{dz}{dx}|_{3D},$$

  where $m$ is a conversion factor and $c$ is the sound speed.

- To be consistent with the pressure and density jump across the shock, the motion of the shock should be matched as well, hence,

$$M_{2D} = m\tan(\beta - \delta).$$

  where $\beta$ is determined by the knowing $M_{3D}$ and the turning angle $\delta$.

Once the conversion factor $m$ is found for a given $M_{3D}, M_{2D}, \delta$, one can compare the 2-D trajectory of the center of mass fraction from the numerical simulation with the 3-D jet lift-off. They find a good agreement for $M_{3D} = 6, \delta = \tan^{-1}(1/12)$ and $M_{2D} = 1.346$, $m = 9.34$. This good agreement indicates that the trajectory of the feature in 2-D corresponds well with the 3-D steady case with the matching of geometry and shock condition.

We solved the two dimensional compressible Navier Stokes equations with three additional equations for the conservation of mass of species in order to take into account of the production of species by the combustion process. A single step reversible chemistry reaction model, namely, $2H_2 + O_2 <=> 2H_2O$ is used. The Soret and Dufour effect, heat radiant effect, pressure gradient diffusion and body force are neglected. The binary coefficient of all species is assumed to be equal and Lewis number $Le = 1$. The mixture viscosity is determined from the Wilke's law. The forward reaction rate of the reaction is given by a modified Arrhenius law.

Two different numerical schemes are used, namely, a spectral scheme [8] and the ENO schemes of Shu and Osher [7]. We begin first by discussing the spectral code in next section.

# 2 Spectral code

- The physical domain of the model is $x \in [0\ cm, 12.5\ cm]$. $y \in [-6.5\ cm, 6.5\ cm]$. The symmetry property of the flow is used for the single jet configuration. This would improve the efficiency for these cases.
- Initially, a Mach 2 normal air shock located at $x = 5\ cm$ and a hydrogen jet of $\approx 2\ cm$ in radius is centered at $x = 2.75\ cm, y = 0\ cm$. The initial temperature of the jet is at 1000 $^oK$ at 1 $atm$.

- Chebyshev collocation methods is used in both $x$ and $y$ directions.

- The Chebyshev collocation points $\xi$ is mapped into another set of interpolation points $x$ by a grid transformation (Kosloff, Tal-Ezer) in the form of

$$x(\xi) = \frac{\sin^{-1}(\alpha\xi)}{\sin^{-1}(\alpha)}$$

  For $\alpha = \text{sech}((\ln\epsilon)/N)$ and $\xi_j = \cos(\pi j/N)$. where $\epsilon$ is the machine zero. CFL number larger than the standard Chebyshev methods would allow can be taken. For $N = 512$, CFL can be 15 times larger using the $x(\xi_j)$ as the interpolation points without any degradation in approximation accuracy.

- Differentiation of the three dimensional data set $(n, m, k)$ is done by applying Cosine Transform-Recursion-Inverse Cosine Transform on the Cray C90. $n, m$ are the number of points in $x$ and $y$, respectively. $k$ is the number of PDE. Typically, $n = m = 512$ and $k = 7$.

- Boundary Condition :
  In the $y$ direction, a reflective boundary condition is used at $y = \pm 6.5\ cm$. Supersonic inflow is imposed on the inflow. At the outflow, characteristic treatment based on the eigenfunctions and eigenvalues of the one dimensional Euler equation is used.

- A low storage third order TVD stable Runge-Kutta scheme (Shu, Osher) is used to march the equations in time. It has the form of

$$\begin{aligned}
\vec{W}^1 &= \vec{W}^n - \Delta t L(\vec{W}^n) \\
\vec{W}^2 &= \frac{1}{4}(3\vec{W}^n + \vec{W}^1 - \Delta t L(\vec{W}^1) \\
\vec{W}^{n+1} &= \frac{1}{3}(\vec{W}^n + 2\vec{W}^2 - 2\Delta t L(\vec{W}^2)
\end{aligned}$$

  where $L$ is the spatial operator for the fluxes.

- At each Runge Kutta time step, the derivative and the solution are filtered by the exponential filter,

$$\sigma(k) = e^{-\alpha(\frac{k}{N})^\gamma}, \quad k = 0, 1, \ldots, N$$

  where $\alpha = -\ln\epsilon$ and $\epsilon$ is the machine zero. Typically, $\gamma = 14$ for the smoothing of the derivative of the fluxes and $\gamma = 12$ for the smoothing of the solution.

  It is mainly used for the purpose of stabilizing the spectral scheme from Gibbs phenomenon and nonlinear instability.

- Gibbs free reconstruction of the data has not yet been implemented in a satisfactory way. Further research is needed.

- At some stage of evolution of the PDE, 1) Gibbs phenomena and/or small scale oscillation in the jets caused negative hydrogen mass fraction, 2) compression of the jets and lack of strong numerical dissipation cause unrealistic local large gradients in species mass fraction. The Global nature of the strong smoothing has the undesirable effect of destroying information in regions other than those few local unstable ones. To deal with kind of situation, points that exceed a certain tolerance level are smoothed locally by nine point averaging. The tolerance is set by limiting the hydrogen mass fraction to not exceed one percent of one below zero. One important point to remember is that the local smoothing is done on the primitive valuables, not on the conservative valuables (does not seem to work well).

## 2.1 Implementation of the spectral code

- The Spectral code is implemented on the Cray C90 at WES High Performance Computing (HPC) Center.
- The code has about 88% of DO loop vectorized.
- The code make used of the multiple fast Fourier Transform routine in the Cray Scientific library to perform the main computational kernel, namely, the differentiation of the fluxes and smoothing of the solution.
- The computational kernel of the algorithm achieves performance of 550 megaflop on a single processor with $512 \times 512$ grids.
- Total CPU time usage for the $512 \times 512$ grids and final phvsical time $T = 80$ microsecond is about $4\frac{1}{2}$ CPU hours. Average CPU for each time step is about 3.8 seconds. Total number of time step is about 4127.

# 3 ENO code

- Geometry same as spectral, except $y \in [0\ cm, 5\ cm]$, using the symmetry property of the flow.
- ENO scheme applied to a regular grid with mappings applied to each coordinate direction separately. uniform grid on $x$, $\tan(\beta x)/c$ in $y$, where $c$ is a constant.
- Boundary Conditions :
  Reflective boundary conditions at $y = 0\ cm$ and $5\ cm$. Characteristic boundary conditions at inflow and outflow.
- The same 3rd order TVD Runge-Kutta applied in the spectral scheme is used to advance in time, using the method of lines.
- Each chemical species is treated as a separate conservative variable in the numerical formulation. Negative species concentrations are treated by clipping values.

- The hyperbolic system is approximately diagonalized locally in order to decouple the system of equations in the ENO derivative. The computed Jacobian matrix includes contributions due to the chemical species, but the dependence of pressure on species mass fraction is ignored.
- Local Lax-Friedrich flux-splitting applied for upwinding.
- Viscosity is computed by central differences. If $s$ is the shu style order of the scheme, up to 2*(s+1) order—user chooses.

### 3.1 ENO Implementation

- The ENO code is implemented on the Thinking Machines CM5 at the Army High Performance Computing Research Center.
- Code implemented using the CMMD message passing library, the CDPEAC **assembly language** and GCC-AC vector C code.
- The algorithm achieves in excess of 1 Gflop on a 32 node machine for $300 \times 300$ grids. On a 512 node machine, the code achieves in excess of 16 Gflops.
- CPU time usage for 10000 time steps for a $1472 \times 736$ grid is about 3 hours for a 512 node machine. 11029 time steps took 10243 seconds (or 2.84 hours). It took 1.58 gigabytes of memory, total.

## 4 Numerical Results

Here we would like to study the resolution properties of the ENO scheme and the spectral scheme for supersonic reactive flows. It is important that the flame front (a narrow region where the combustion take place) to be well resolved. The physical aspect of this problem will be study in some later time. Hence, to simplify the number of PDE to be solved, we solved the Euler equation without combustion. (ENO version of the full combustion model is under development. The spectral version of the full combustion model is ready and running.)

The 2D supersonic reactive flow is modeled by a Mach 2 normal air shock moving toward right side of the domain and interacted with a column of hydrogen jet as depicted in figure 1. (Solution for multiple hydrogen jets configuration is also available).

The hydrogen mass fraction of the second order ENO scheme (Shu's definition) with grid size $240 \times 120$, and $1472 \times 736$ are shown in figures 2 and 3 respectively. at $t = 60$ microsecond. The corresponding solution from the spectral code with grid size $512 \times 512$ is shown in figure 5. The global structure (for example, density) of the two algorithms is very similar. The fine structures (for example, the flame front), however, was not captured in the low resolution version of the ENO scheme. In most literature, this is the solution that other researches (FCT, ENO) had obtained. As the resolution of the ENO scheme increased, it then able to capture the finer structure inside the hydrogen jet. Still, the strong inherent numerical

dissipation of the scheme prevented further development of some finer structures in later time. The spectral solution, however, shows a great deal more structures. More noticeably is the mushroom shape structure which is a tell-tale sign of Rayleigh-Taylor instability.

A third order ENO scheme was developed with mapping to cluster points near the jet. The hydrogen mass fraction now indicate a completely new configuration inside the hydrogen jet than the low resolution case (figure 5). A mushroom shape structure is now emerged from where the air penetrating the hydrogen (A Rayleigh-Taylor instability). The important of high-order/high resolution scheme in resolving the combustion front is evident from this study.

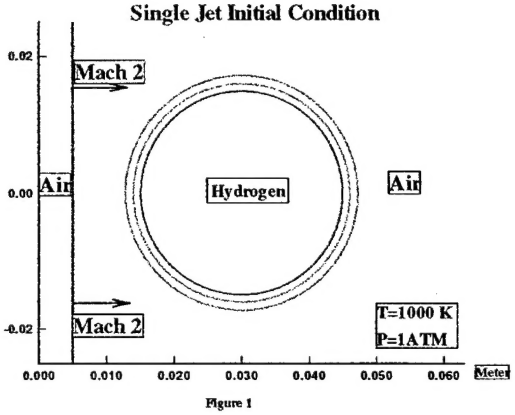

Figure 1

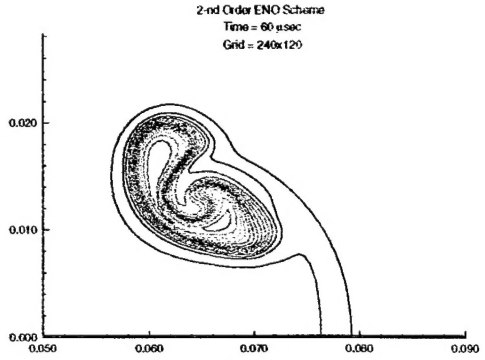

Figure 2

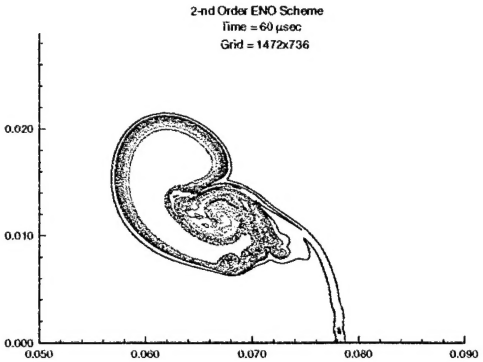

Figure 3

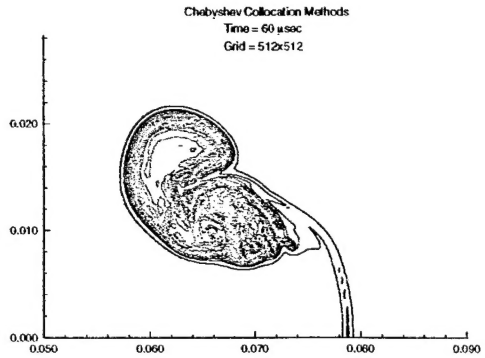

Figure 4

# References


[1] J. P. Boris, D. L. Book, *Flux-Corrected Transport I : SHASTA - A Fluid Transport Algorithm that Works*, J. Comp. Physics, **11** (1973), p. 38-69

[2] F. E. Marble *Growth of a Diffusion Flame in the Field of a Vortex.* In **Recent Advances in the Aerospace Sciences** (ed. Corrado Casci), pp. 395–412

[3] F. E. Marble, E. E. Zukoski, J. W. Jacobs, G. J. Hendricks. I. A. Waitz, *Shock Enhancement and Control of Hypersonic Mixing and Combustion.* AIAA Paper 90-1981

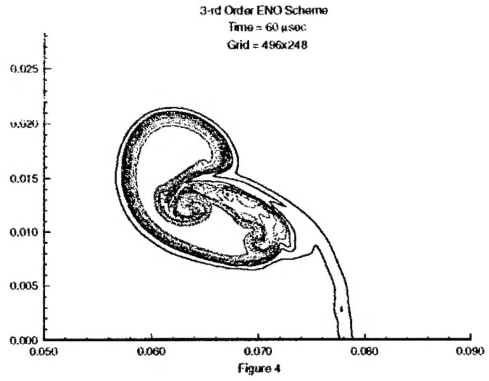

Figure 4

[4] J. M. Picone and J. P. Boris, *Vorticity generation by shock propagation through bubbles in a gas* J. Fluid Mech., **189**, pp 23–51

[5] J. Yang, T. Kubota, E. E. Zukoski, *A model for characterization of a vortex pair formed by shock passage over a light gas inhomogeneity*, J. Fluid Mech., **258** (1994), pp. 217–244

[6] V. T. Ton *A numerical Method for Mixing/Chemically Reacting Compressible Flow with Finite Rate Chemistry* Ph.D. thesis, UCLA, 1993

[7] C. W. shu and S. J. Osher, *Efficient Implementation of Essentially Non-Oscillatory Shock-Capturing Schemes, II,"* J. Comput. Phys., **83**, pp 32–78

[8] W. S. Don *Numerical study of pseudospectral methods in shock wave applications*, J. Comp. Physics **110** (1994),, pp. 103–111